The Mystery of the Shape Parameter IV

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Abstract. This is the fourth paper of our study of the shape parameter c contained in the famous multiquadrics $(-1)^{\lceil\beta\rceil}(c^2+\|x\|^2)^\beta,\ \beta>0$, and the inverse multiquadrics $(c^2+\|x\|^2)^\beta,\ \beta<0$. The theoretical ground is the same as that of [10]. However we extend the space of interpolated functions to a more general one. This leads to a totally different set of criteria of choosing c.

keywords: radial basis function, multiquadric, shape parameter, interpolation.

1 Introduction

Again, we are going to adopt the radial function

$$h(x) := \Gamma(-\frac{\beta}{2})(c^2+|x|^2)^{\frac{\beta}{2}},\ \beta\in R\backslash 2N_{\geq 0},\ c>0 \tag{1}$$

, where $|x|$ is the Euclidean norm of x in R^n, Γ is the classical gamma function, and c,β are constants. This definition looks more complicated than the ones mentioned in the abstract. However it will simplify the Fourier transform of h and our analysis of some useful results.

In order to make this paper more readable, we review some basic ingredients mentioned in the previous papers, at the cost of wasting a few pages.

For any interpolated function f, our interpolating function will be of the form

$$s(x) := \sum_{i=1}^{N} c_i h(x-x_i)+p(x) \tag{2}$$

where $p(x)\in P_{m-1}$, the space of polynomials of degree less than or equal to $m-1$ in $R^n, X=\{x_1,\cdots,x_N\}$ is the set of centers(interpolation points). For $m=0,\ P_{m-1}:=\{0\}$. We require that $s(\cdot)$ interpolate $f(\cdot)$ at data points $(x_1,f(x_1)),\cdots,(x_N,f(x_N))$. This results in a linear system of the form

$$\sum_{i=1}^{N} c_i h(x_j-x_i)+\sum_{i=1}^{Q} b_i p_i(x_j)=f(x_j) \qquad ,j=1,\cdots,N \tag{3}$$

$$\sum_{i=1}^{N} c_i p_j(x_i) = 0 \qquad , j = 1, \cdots, Q$$

to be solved, where $\{p_1, \cdots, p_Q\}$ is a basis of P_{m-1}.

This linear system is solvable because $h(x)$ is conditionally positive definite(c.p.d.) of order $m = max\{\lceil \frac{\beta}{2} \rceil, 0\}$ where $\lceil \frac{\beta}{2} \rceil\}$ denotes the smallest integer greater than or equal to $\frac{\beta}{2}$.

Besides the linear system, another important object is the function space. Each function of the form (1) induces a function space called **native space** denoted by $\mathcal{C}_{h,m}(R^n)$, abbreviated as $\mathcal{C}_{h,m}$, where m denotes its order of conditional positive definiteness. For each member f of $\mathcal{C}_{h,m}$ there is a seminorm $\|f\|_h$, called the h-norm of f. The definition and characterization of the native space can be found in [4], [5], [7], [11], [12] and [14]. In this paper all interpolated functions belong to the native space.

Although our interpolated functions are defined in the entire R^n, interpolation will occur in a simplex. The definition of simplex can be found in [3]. A 1-simplex is a line segment, a 2-simplex is a triangle, and a 3-simplex is a tetrahedron with four vertices.

Let T_n be an n-simplex in R^n and $v_i,\ 1 \le i \le n+1$ be its vertices. Then any point $x \in T_n$ can be written as convex combination of the vertices:

$$x = \sum_{i=1}^{n+1} c_i v_i,\ \sum_{i=1}^{n+1} c_i = 1,\ c_i \ge 0.$$

The numbers $c_1, \cdots, c_{n+1}$ are called the barycentric coordinates of x. For any n-simplex T_n, the **evenly spaced points** of degree l are those points whose barycentric coordinates are of the form

$$(\frac{k_1}{l}, \frac{k_2}{l}, \cdots, \frac{k_{n+1}}{l}),\ k_i\ nonnegative\ integers\ with\ \sum_{i=1}^{n+1} k_i = l.$$

It's easily seen that the number of evenly spaced points of degree l in T_n is exactly

$$N = dimP_l^n = \begin{pmatrix} n+l \\ n \end{pmatrix}$$

where P_l^n denotes the space of polynomials of degree not exceeding l in n variables. Moreover, such points form a determining set for P_l^n, as is shown in [2].

In this paper the evaluation argument x will be a point in an n-simplex, and the set X of centers will be the evenly spaced points in that n-simplex.

2 Fundamental Theory

Before introducing the main theorem, we need to define two constants.

Definition 2.1 *Let n and β be as in (1). The numbers ρ and Δ_0 are defined as follows.*

(a) Suppose $\beta < n-3$. Let $s = \lceil \frac{n-\beta-3}{2} \rceil$. Then

(i) if $\beta < 0,\ \rho = \frac{3+s}{3}$ and $\Delta_0 = \frac{(2+s)(1+s)\cdots 3}{\rho^2}$;

(ii) if $\beta > 0,\ \rho = 1 + \frac{s}{2\lceil \frac{\beta}{2} \rceil + 3}$ and $\Delta_0 = \frac{(2m+2+s)(2m+1+s)\cdots(2m+3)}{\rho^{2m+2}}$ where $m = \lceil \frac{\beta}{2} \rceil$.

(b) *Suppose* $n-3 \le \beta < n-1$. *Then* $\rho = 1$ *and* $\Delta_0 = 1$.

(c) *Suppose* $\beta \ge n-1$. *Let* $s = -\lceil \frac{n-\beta-3}{2} \rceil$. *Then*

$$\rho = 1 \text{ and } \Delta_0 = \frac{1}{(2m+2)(2m+1)\cdots(2m-s+3)} \text{ where } m = \lceil \frac{\beta}{2} \rceil.$$

The following theorem is the cornerstone of our theory. We cite it directly from [6] with a slight modification to make it easier to understand.

Theorem 2.2 *Let* h *be as in (1). For any positive number* b_0, *let* $C = \max\left\{\frac{2}{3b_0}, 8\rho\right\}$ *and* $\delta_0 = \frac{1}{3C}$. *For any* n*-simplex* Q *of diameter* r *satisfying* $\frac{1}{3C} \le r \le \frac{2}{3C}$ *(note that* $\frac{2}{3C} \le b_0$*), if* $f \in \mathcal{C}_{h,m}$,

$$|f(x) - s(x)| \le 2^{\frac{n+\beta-7}{4}} \pi^{\frac{n-1}{4}} \sqrt{n\alpha_n} c^{\frac{\beta}{2}-l} \sqrt{\Delta_0} \sqrt{3C} \sqrt{\delta} (\lambda')^{\frac{1}{\delta}} \|f\|_h \tag{4}$$

holds for all $x \in Q$ *and* $0 < \delta < \delta_0$, *where* $s(x)$ *is defined as in (2) with* $x_1, \cdots, x_N$ *the evenly spaced points of degree* l *in* Q *satisfying* $\frac{1}{3C\delta} \le l \le \frac{2}{3C\delta}$. *The constant* α_n *denotes the volume of the unit ball in* R^n, *and* $0 < \lambda' < 1$ *is given by*

$$\lambda' = \left(\frac{2}{3}\right)^{\frac{1}{3C}}$$

which only in some cases mildly depends on the dimension n.

Remark:(a)Note that the right-hand side of (4) approaches zero as $\delta \to 0^+$. This is the key to understanding Theorem2.2. The number δ is in spirit equivalent to the well-known fill-distance. Although the centers $x_1, \cdots, x_N$ are not purely scattered, the shape of the simplex is controlled by us. Hence the distribution of the centers is practically quite flexible. (b)In (4) the shape parameter c plays a crucial role and greatly influences the error bound. This provides us with a theoretical ground of choosing the optimal c. However we need further work before presenting useful criteria.

In this paper all interpolated functions belong to a kind of space defined as follows.

Definition 2.3 *For any positive number* σ,

$$E_\sigma := \left\{ f \in L^2(R^n) : \int |\hat{f}(\xi)|^2 e^{\frac{|\xi|^2}{\sigma}} d\xi < \infty \right\}$$

where $\hat{f}$ *denotes the Fourier transform of* f. *For each* $f \in E_\sigma$, *its norm is*

$$\|f\|_{E_\sigma} := \left\{ \int |\hat{f}(\xi)|^2 e^{\frac{|\xi|^2}{\sigma}} d\xi \right\}^{1/2}$$

.

The following lemma is cited from [9].

Lemma 2.4 *Let* h *be as in (1). For any* $\sigma > 0$, *if* $\beta < 0$, $|n+\beta| \ge 1$ *and* $n+\beta+1 \ge 0$, *then* $E_\sigma \subseteq \mathcal{C}_{h,m}(R^n)$ *and for any* $f \in E_\sigma$, *the seminorm* $\|f\|_h$ *of* f *satisfies*

$$\|f\|_h \le 2^{-n-\frac{1+\beta}{4}} \pi^{-n-\frac{1}{4}} c^{\frac{1-n-\beta}{4}} \left\{ (\xi^*)^{\frac{n+\beta+1}{2}} e^{c\xi^* - \frac{(\xi^*)^2}{\sigma}} \right\}^{1/2} \|f\|_{E_\sigma}$$

where

$$\xi^* := \frac{c\sigma + \sqrt{c^2\sigma^2 + 4\sigma(n+\beta+1)}}{4}$$

.

Corollary 2.5 *Under the conditions of Theorem2.2, if $f \in E_\sigma,\ \beta < 0,\ |n+\beta| \geq 1$ and $n+\beta+1 \geq 0$, (4) can be transformed into*

$$|f(x) - s(x)| \leq 2^{-\frac{3n}{4}-2}\pi^{-\frac{3}{4}n-\frac{1}{2}}\sqrt{n\alpha_n}\sqrt{\Delta_0}\sqrt{3C}c^{\frac{\beta-n+1-4l}{4}}\left\{(\xi^*)^{\frac{n+\beta+1}{2}}e^{c\xi^*-\frac{(\xi^*)^2}{\sigma}}\right\}^{1/2}\sqrt{\delta}(\lambda')^{\frac{1}{\delta}}\|f\|_{E_\sigma} \quad (5)$$

where

$$\xi^* := \frac{c\sigma + \sqrt{c^2\sigma^2 + 4\sigma(n+\beta+1)}}{4}$$

.

Proof. This is an immediate result of Theorem2.2 and Lemma2.4. ♯

Note that Corollary2.5 covers the very useful case $\beta = -1,\ n \geq 2$. However the case $\beta = -1,\ n = 1$ is excluded. For this case we need a different approach.

Lemma 2.6 *Let $\sigma > 0,\ \beta = -1$ and $n = 1$. For any $f \in E_\sigma$,*

$$\|f\|_h \leq 2^{-(n+\frac{1}{4})}\pi^{-1}\left\{\frac{1}{ln2} + 2\sqrt{3}M(c)\right\}^{1/2}\|f\|_{E_\sigma}$$

where $M(c) := e^{1-\frac{1}{c^2\sigma}}$ if $c \leq \frac{2}{\sqrt{3\sigma}}$ and $M(c) := g(\frac{c\sigma+\sqrt{c^2\sigma^2+4\sigma}}{4})$ if $c > \frac{2}{\sqrt{3\sigma}}$, where $g(\xi) := \sqrt{c\xi}e^{c\xi-\frac{\xi^2}{\sigma}}$.

Proof. This is just Theorem2.5 of [9]. ♯

Corollary 2.7 *Let $\sigma > 0,\ \beta = -1$ and $n = 1$. Under the conditions of Theorem2.2, if $f \in E_\sigma$, (4) can be transformed into*

$$|f(x) - s(x)| \leq 2^{\frac{\beta-3n}{4}-2}\pi^{\frac{n-5}{4}}\sqrt{n\alpha_n}\sqrt{\Delta_0}\sqrt{3C}c^{\frac{\beta}{2}-l}\left\{\frac{1}{ln2} + 2\sqrt{3}M(c)\right\}^{1/2}\sqrt{\delta}(\lambda')^{\frac{1}{\delta}}\|f\|_{E_\sigma} \quad (6)$$

where $M(c)$ is defined as in Lemma2.6.

Proof. This is an immediate result of Theorem2.2 and Lemma2.6. ♯

Now we have dealt with the most useful cases for $\beta < 0$. The next step is to treat $\beta > 0$.

Lemma 2.8 *Let $\sigma > 0,\ \beta > 0$ and $n \geq 1$. For any $f \in E_\sigma$,*

$$\|f\|_h \leq d_0 c^{\frac{1-\beta-n}{4}}\left\{\frac{(\xi^*)^{\frac{1+\beta+n}{2}}e^{c\xi^*}}{e^{\frac{(\xi^*)^2}{\sigma}}}\right\}^{1/2}\|f\|_{E_\sigma}$$

where $\xi^* = \frac{c\sigma+\sqrt{c^2\sigma^2+4\sigma(1+\beta+n)}}{4}$ and d_0 is a constant depending on $n,\ \beta$ only.

Proof. This is just Theorem2.8 of [9]. ♯

Corollary 2.9 *Let $\sigma > 0,\ \beta > 0$ and $n \geq 1$. If $f \in E_\sigma$, (4) can be transformed into*

$$|f(x) - s(x)| \leq 2^{\frac{n+\beta-7}{4}}\pi^{\frac{n-1}{4}}\sqrt{n\alpha_n}\sqrt{\Delta_0}\sqrt{3C}d_0 c^{\frac{1+\beta-n-4l}{4}}\left\{\frac{(\xi^*)^{\frac{1+\beta+n}{2}}e^{c\xi^*}}{e^{\frac{(\xi^*)^2}{\sigma}}}\right\}^{1/2}\sqrt{\delta}(\lambda')^{\frac{1}{\delta}}\|f\|_{E_\sigma} \quad (7)$$

where $d_0,\ \xi^*$ are as in Lemma2.8.

Proof. This is an immediate result of Theorem2.2 and Lemma2.8. ♯

3 Criteria of Choosing c

Note that in (5),(6) and (7), there is a main function of c. As in [9], let's call this function the MN function, denoted by $MN(c)$, and its graph the MN curve. The optimal choice of c is then the number minimizing $MN(c)$. However, unlike [9], the range of c is the entire interval $(0,\infty)$, rather than a proper subset of $(0,\infty)$.

We now begin our criteria.

Case1. $\boxed{\beta < 0,\ |n+\beta| \geq 1 \text{ and } n+\beta+1 \geq 0}$ Let $f \in E_\sigma$ and h be as in (1). Under the conditions of Theorem2.2, for any fixed δ satisfying $0 < \delta < \delta_0$, the optimal value of c in $(0,\infty)$ is the number minimizing

$$MN(c) := c^{\frac{\beta-n+1-4l}{4}} \left\{ (\xi^*)^{\frac{n+\beta+1}{2}} e^{c\xi^* - \frac{(\xi^*)^2}{\sigma}} \right\}^{1/2}$$

where

$$\xi^* = \frac{c\sigma + \sqrt{c^2\sigma^2 + 4\sigma(n+\beta+1)}}{4}$$

.

Reason: This is a direct consequence of (5). ♯

Remark:(a)It's easily seen that $MN(c) \to \infty$ as $c \to \infty$. Also, if $n+\beta+1 > 0$, $MN(c) \to \infty$ as $c \to 0^+$. (b)Case1 covers the frequently seen case $\beta = -1$, $n \geq 2$. (c)The number c minimizing $MN(c)$ can be easily found by Mathematica or Matlab.

Numerical Results:

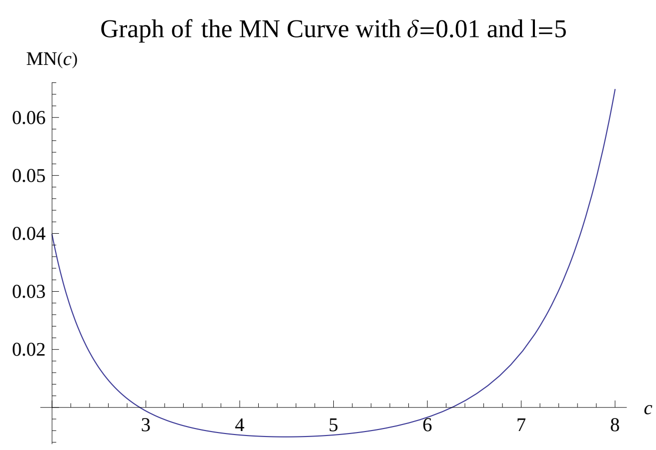

Figure 1: Here $n = 2, \beta = -1, \sigma = 1$ and $b_0 = 1$.

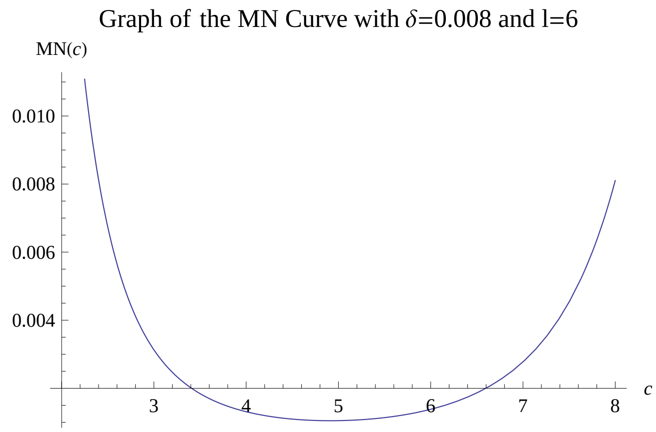

Figure 2: Here $n = 2, \beta = -1, \sigma = 1$ and $b_0 = 1$.

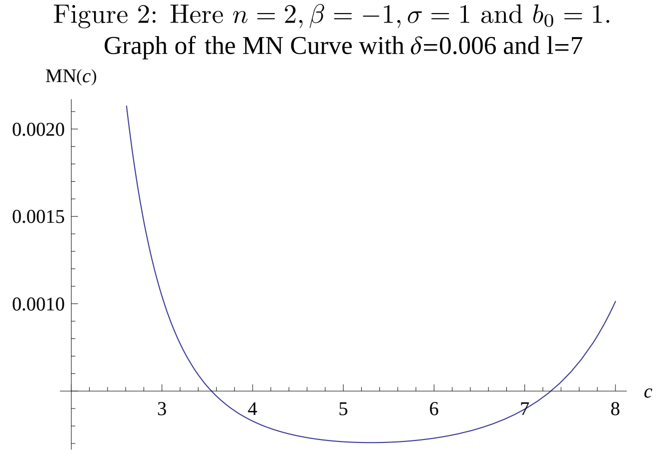

Figure 3: Here $n = 2, \beta = -1, \sigma = 1$ and $b_0 = 1$.

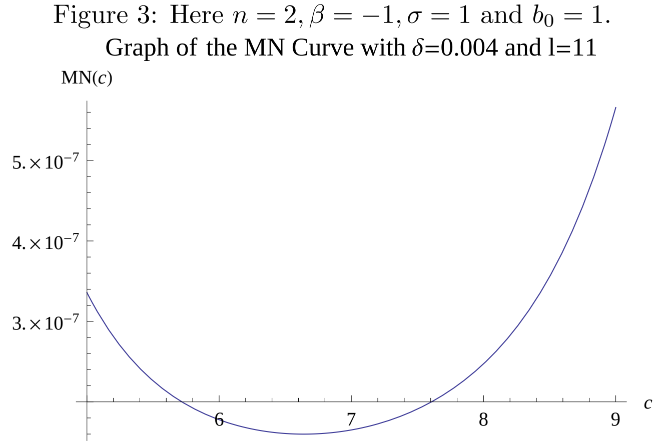

Figure 4: Here $n = 2, \beta = -1, \sigma = 1$ and $b_0 = 1$.

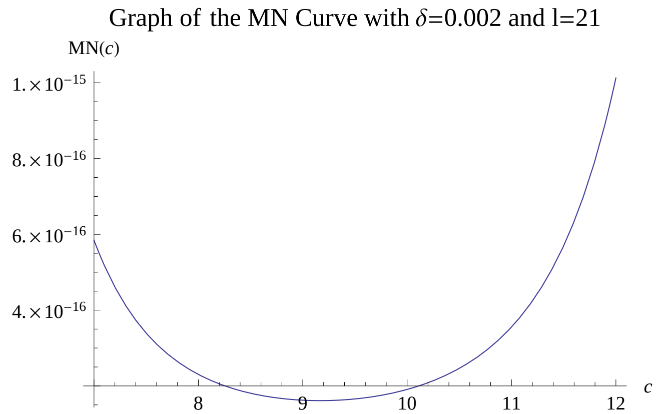

Figure 5: Here $n = 2, \beta = -1, \sigma = 1$ and $b_0 = 1$.

Case2. $\boxed{\beta = -1 \text{ and } n = 1}$ Let $f \in E_\sigma$ and h be as in (1). Under the conditions of Theorem2.2, for any fixed δ satisfying $0 < \delta < \delta_0$, the optimal value of c in $(0, \infty)$ is the number minimizing

$$MN(c) := c^{\frac{\beta}{2}-l}\left\{\frac{1}{ln2} + 2\sqrt{3}M(c)\right\}^{1/2}$$

where

$$M(c) := \begin{cases} e^{1-\frac{1}{c^2\sigma}} & \text{if } 0 < c \le \frac{2}{\sqrt{3\sigma}}, \\ g\left(\frac{c\sigma+\sqrt{c^2\sigma^2+4\sigma}}{4}\right) & \text{if } \frac{2}{\sqrt{3\sigma}} < c \end{cases}$$

, g being defined by $g(\xi) := \sqrt{c\xi}e^{c\xi-\frac{\xi^2}{\sigma}}$.

Reason: This is a direct result of (6). $\sharp$

Remark: Note that $MN(c) \to \infty$ both as $c \to \infty$ and $c \to 0^+$. Now let's see some numerical examples.

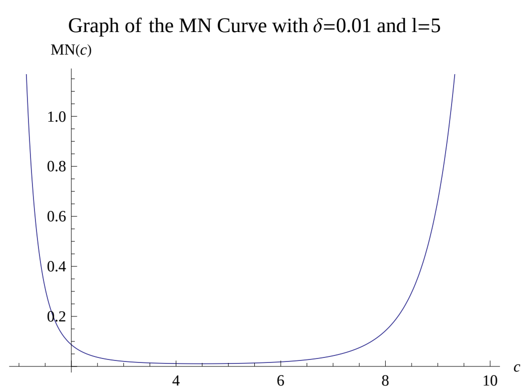

Figure 6: Here $n = 1, \beta = -1, \sigma = 1$ and $b_0 = 1$.

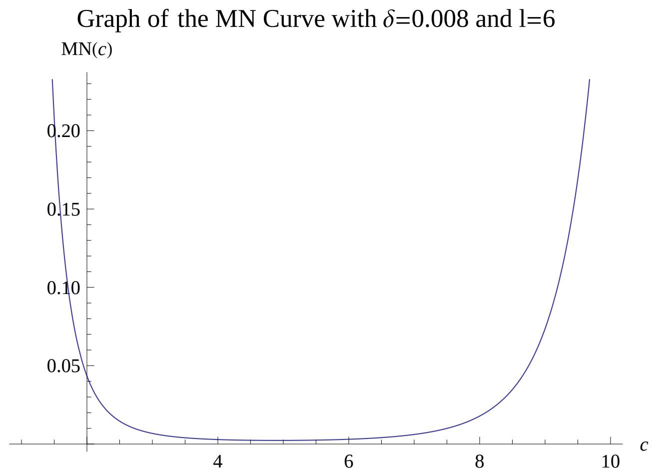

Figure 7: Here $n = 1, \beta = -1, \sigma = 1$ and $b_0 = 1$.

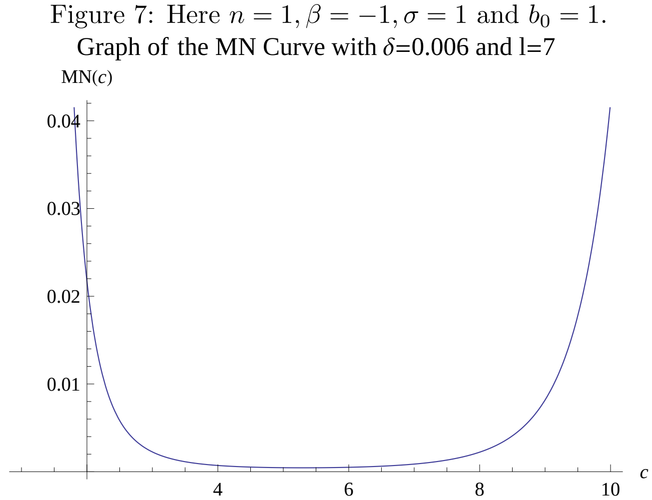

Figure 8: Here $n = 1, \beta = -1, \sigma = 1$ and $b_0 = 1$.

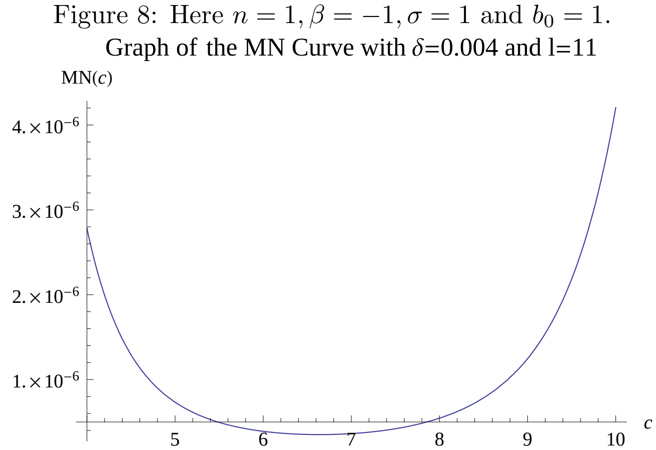

Figure 9: Here $n = 1, \beta = -1, \sigma = 1$ and $b_0 = 1$.

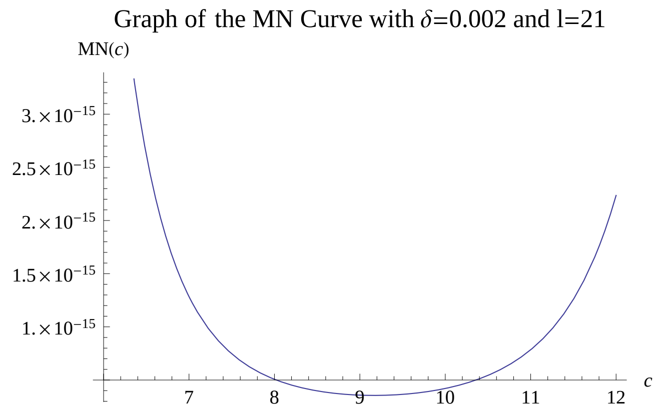

Figure 10: Here $n = 1, \beta = -1, \sigma = 1$ and $b_0 = 1$.

Case3. $\boxed{\beta > 0 \text{ and } n \geq 1}$ Let $f \in E_\sigma$ and h be as in (1). Under the conditions of Theorem2.2, for any fixed δ satisfying $0 < \delta < \delta_0$, the optimal value of c in $(0, \infty)$ is the number minimizing

$$MN(c) := c^{\frac{1+\beta-n-4l}{4}} \left\{ \frac{(\xi^*)^{\frac{1+\beta+n}{2}} e^{c\xi^*}}{e^{\frac{(\xi^*)^2}{\sigma}}} \right\}^{1/2}$$

, where

$$\xi^* = \frac{c\sigma + \sqrt{c^2\sigma^2 + 4\sigma(1+\beta+n)}}{4}$$

.

Reason: This follows from (7). ♯

Remark: By observing that

$$c\xi^* - \frac{(\xi^*)^2}{\sigma} = \frac{1}{16}\left[2c^2\sigma + 2c\sqrt{c^2\sigma^2 + 4\sigma(n+\beta+1)} - (4n+\beta+1)\right]$$

, we can easily obtain useful results as follows. (a)If $1+\beta-n-4l > 0$, $\lim_{c\to 0^+} MN(c) = 0$. (b)If $1+\beta-n-4l < 0$, $\lim_{c\to 0^+} MN(c) = \infty$. (c)If $1+\beta-n-4l = 0$, $\lim_{c\to 0^+} MN(c)$ is a finite positive number. (d)$\lim_{c\to\infty} MN(c) = \infty$.

Numerical Results: For simplicity, we offer results for $n = 1$ only. In fact for $n \geq 1$ similar results can be presented without slight difficulty.

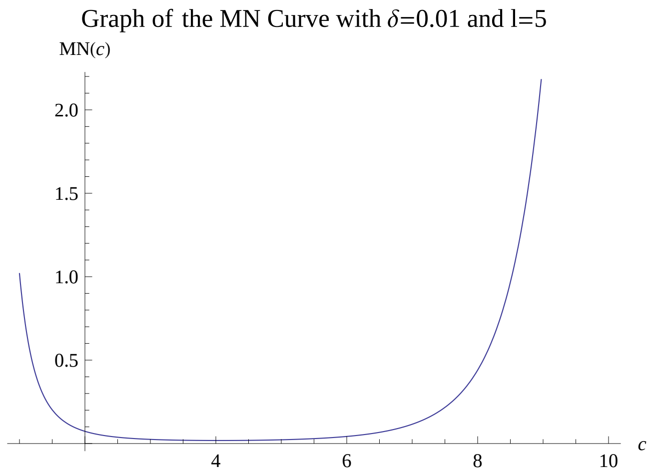

Figure 11: Here $n = 1, \beta = 1, \sigma = 1$ and $b_0 = 1$.

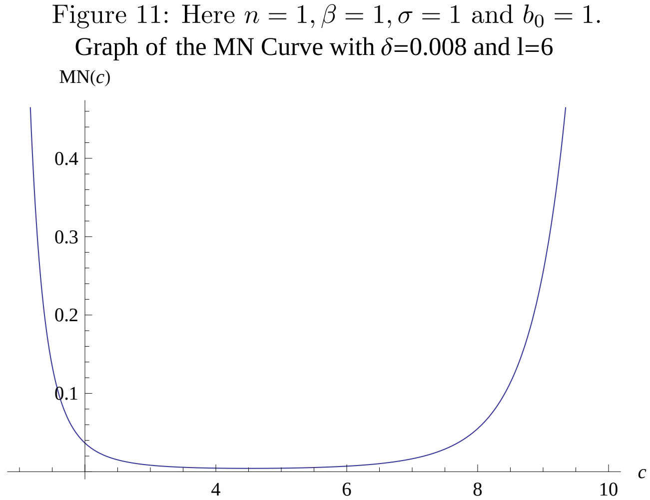

Figure 12: Here $n = 1, \beta = 1, \sigma = 1$ and $b_0 = 1$.

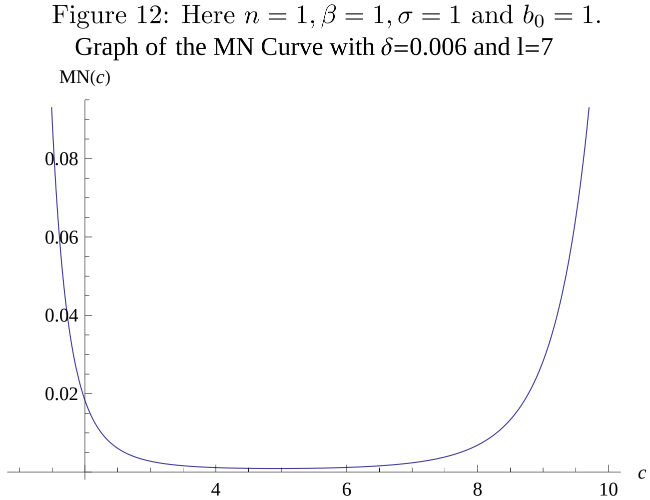

Figure 13: Here $n = 1, \beta = 1, \sigma = 1$ and $b_0 = 1$.

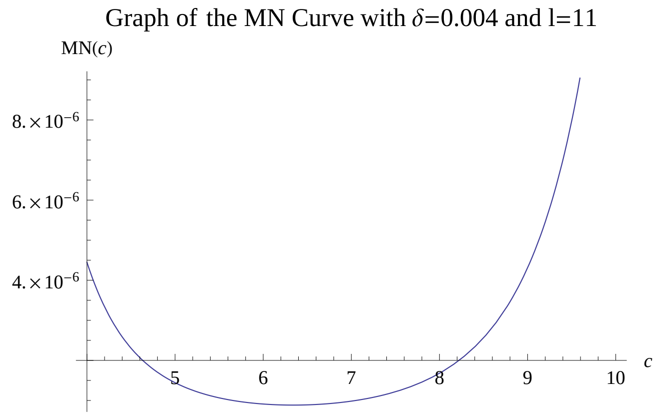

Figure 14: Here $n = 1, \beta = 1, \sigma = 1$ and $b_0 = 1$.

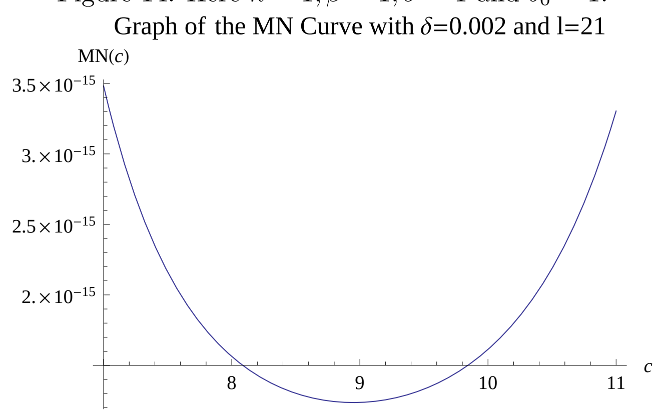

Figure 15: Here $n = 1, \beta = 1, \sigma = 1$ and $b_0 = 1$.

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